

TOXNET:

Toxicology & Environmental Information

http://toxnet.nlm.nih.gov/



TOXNET - Databases on toxicology, hazardous chemicals, environmental health, and toxic releases.



National Network of Libraries of Medicine, South Central Region Houston Academy of Medicine-Texas Medical Center Library 1133 John Freeman Blvd. Houston, TX 77030

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TOXNET (<u>TOX</u>icology Data <u>NET</u>work)

http://toxnet.nlm.nih.gov/

- A FREE web-based integrated system of databases on toxicology, environmental health, hazardous chemicals, toxic releases, chemical nomenclature, and specialty areas such as occupational health and consumer products
- A product of NLM's Toxicology and Environmental Health Information Program (TEHIP)

Five Types of Databases

- Chemical Information: ChemIDplus
- 2. Toxicology <u>Data</u> Files (one record per chemical):
 - a. HSDB
 - b. CCRIS
 - c. GENE-TOX
 - d. IRIS
 - e. ITER
 - f. LactMed
- 3. Toxicology <u>Literature</u> Files (bibliographic references):
 - a. TOXLINE
 - b. DART
- 4. Toxic <u>Releases</u> (chemicals into the environment)
 - a. TRI
 - b. TOXMAP
- 5. Other Databases:
 - a. Haz-Map
 - b. Household Products

Select Database	
• ChemIDplus	?
• HSDB	?
TOXLINE	?
• CCRIS	?
• DART	?
GENETOX	?
• IRIS	?
• ITER	?
LactMed	?
Multi-Database	?
• TRI	?
• Haz-Map	?
Household Products	?
• TOXMAP	?

TOXNET Data Files

Hazardous Substances Data Bank (HSDB)

- From NLM
- Over 5,000 chemical records
- Toxicology of potentially hazardous chemicals
- Information on human exposure, industrial hygiene, emergency handling procedures, environmental fate and regulatory requirements
- Data from books, government documents, technical reports and selected primary literature
- Some data is compiled expressly for HSDB
- Peer reviewed by the Scientific Review Panel

Chemical Carcinogenesis Research Information System (CCRIS)

- From the National Cancer Institute (NCI)
- Over 9,000 chemical records
- Data and information on carcinogenicity, mutagenicity, tumor promotion, and tumor inhibition test results
- Data derived from studies cited in primary journals, current awareness tools, NCI reports, and other special sources
- Scientifically evaluated and fully referenced

Genetic Toxicology (GENE-TOX)

- From the U.S. Environmental Protection Agency (EPA)
- Note: GENE-TOX not updated since January 2000
- 3,214 Chemical Records
- Mutagenicity studies
- Data Structure assay type, assay code, results, panel report, reference
- Selected literature was reviewed by scientific experts

Integrated Risk Information System (IRIS)

- From the EPA
- Contains EPA consensus scientific positions and quantitative values on cancer and non-cancer health effects that may result from lifetime oral or inhalation exposure to specific chemical substances in the environment
- About 550 chemical records
- Scientifically reviewed by groups of EPA scientists and represent EPA consensus

International Toxicity Estimates for Risk Assessment (ITER)

- From Toxicology Excellence for Risk Assessment (TERA), a non-profit corporation
- Provides a comparison of international risk assessment information derived by different organizations (U.S. and International)

- About 650 chemical records
- Includes synopses, links to organization source documents

LactMed

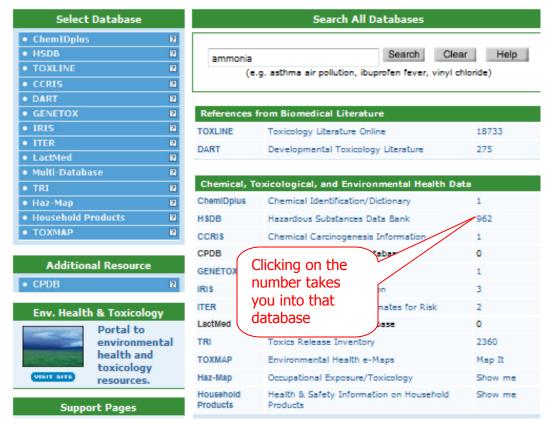
- From NLM
- Database of drugs and other chemicals to which breastfeeding mothers may be exposed and the possible effects in nursing infants
- About 800 records
- Peer-reviewed and fully referenced

Searching TOXNET

- Each TOXNET database may be searched individually or by using the Search
 All Databases option (record counts may vary somewhat when databases
 are searched individually)
- The databases employ very similar search engines. Search techniques for Search All Databases can be used for each database

Searching All Databases

- Search by chemical names, other terms (including multiple terms), and numbers (including CAS numbers)
- Search results display a summary of the number of records retrieved in each database



TOXNET Data Files

Example: HSDB (Hazardous Substances Data Bank)

		TOXNET		THE PERSON NAMED IN	
	NLM	Toxicology Data N	etwork		
			Home About U	s Site Map & Search	Contact Us
Save Checked Items	HSDB S	earch Results	·	Env. Health & Toxicology	TOXNET ▶ HSDI
Sort	ammonia	Searc	ch Clear	Limits	
Details	For chemic	als, add synonyms and CAS num	bers to search:	Yes No	
History	Items 1 thro	ugh 20 of 962	Page 1	1 of 49. Go to page	>
Download	Substance I	Names are sorted in <u>relevancy rank</u>	<u>ked</u> order.		
Modify Search	Select Record	Substance Name			
Basic Search	The followin	g is the primary record for the che	Click on ch	emical found.	
Browse Index		AMMONIA 7664-41-7	name to ac full record	ccess	
Help		g 961 records contain one or more		hemical name(s) and all o	f the query
TOXNET Home		here in the record.	or the requested e		- and quary
		AMMONIUM HYDROXIDE 1336-21-6			

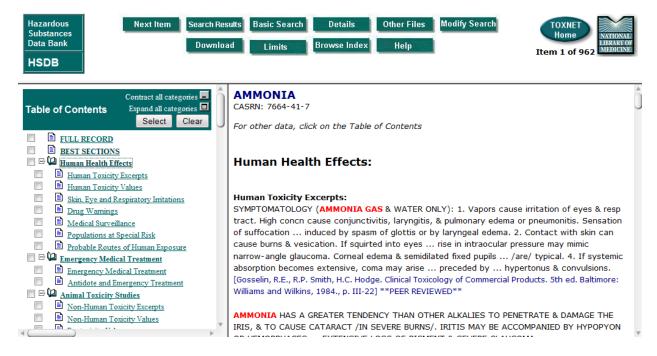
Results display best matches first



- **Saved Checked Items** option allows you to display selected records only
 - Check box next to record number(s)
 - Click Saved Checked Items
 - Click **Display Saved Items** to view only the selected records (this option is only displayed when records are selected)
- **Sort** allows selected records to be resorted in ascending or descending order. TIP: This is best used with **Saved Checked Items**
- Details displays the search strategy
- **History** displays your recent searches
- Download allows some or all of the records retrieved to be downloaded in brief or full format. TIP: This is best used with Saved Checked Items
- Browse Index opens the Browse the Index search screen

Full Record Display

 The Full Record Display for each TOXNET data file has a similar look and navigation



- The search term(s) is highlighted in red in the full record
- Each database has the **Table of Contents** in the left frame and the full record in the right frame
- The **Table of Contents** includes quick links to the specific fields and categories within the record. Links include:
 - Human Health Effects (which is the default display in HSDB)
 - Emergency Medical Treatment
 - Animal Toxicity Studies
 - Environmental Fate and Exposure
 - Manufacturing/Use Information (includes the major uses of the substance and manufacturers)

Moving between Databases

 The Other Files button, located at the top of the results page, allows the search to be conducted in other TOXNET files



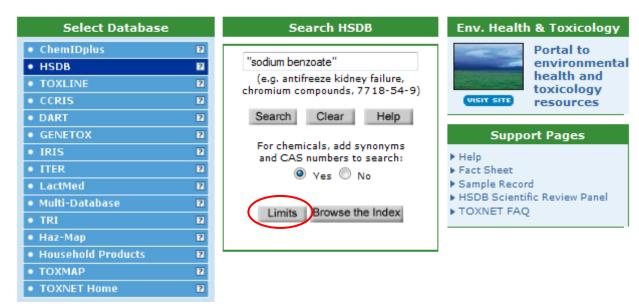
Advanced Searching

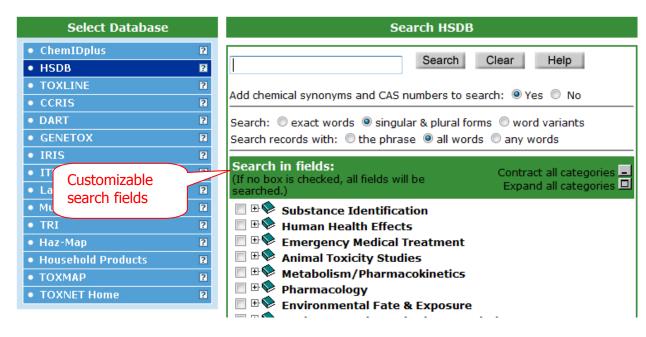
- Boolean searching using AND, OR, and NOT is available
- Truncation using the asterisk (*) is allowed at the end of a word and will search any number of characters
- Phrase searching by quotation marks is allowed

Searching Individual Databases

Clicking on the **Limits** button allows you to search specific fields in the record

Hazardous Substances Data Bank (HSDB) - Comprehensive, peer-reviewed toxicology data for about 5,000 chemicals.





Practice Exercises

1. What are the adverse effects of exposure to phenol?

2. What is lithium chromate used for?

3. Is coal tar a carcinogen?

TOXNET Literature Files

TOXLINE (TOXicology Literature onLINE)

- Bibliographic information on pharmacological, biochemical, physiological, environmental, and toxicological effects of chemicals and other agents on living systems
- Sources of information include: toxicology journals, technical reports, research projects and archival collections
- Over 4 million citations
- Links to PubMed citations

Developmental and Reproductive Toxicology/Environmental Teratology Information Center (DART/ETIC)

- Managed by NLM and funded by the EPA, the National Institute of Environmental Health Sciences (NIEHS), the National Center for Toxicological Research (NCTR) of the Food and Drug Administration (FDA), and NLM
- Bibliographic information on teratology and other aspects of developmental and reproductive toxicology
- Over 200,000 citations
- Links to PubMed citations

Searching TOXLINE

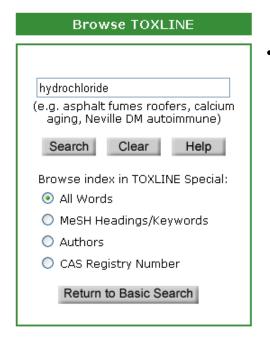
 NOTE: TOXLINE and DART employ very similar search engines. All search techniques for TOXLINE can be used for DART



Toxicology Literature Online (TOXLINE) - References from toxicology literature.

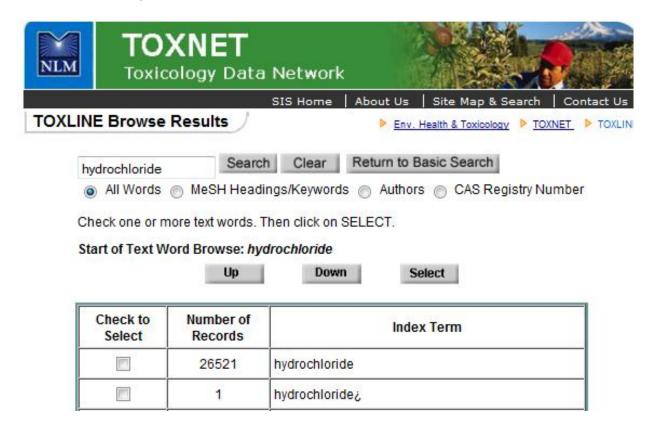


- Search by chemical names, other terms (including multiple terms), and numbers (including CAS numbers)
- Adding synonyms and CAS numbers expands your search results.
- Including PubMed citations in the results is optional

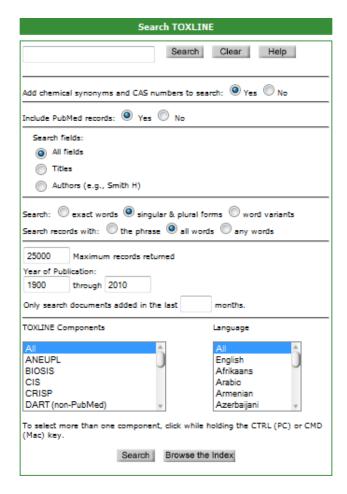


Browse the Index allows browsing by terms, MeSH headings or Keywords, Authors or CAS number

- Review the results in the index
 - Check the appropriate term and click Select to retrieve citation results
- Click on the Up or Down button to scan the results



- Click on the **Limits** button to limit your search. Type of **Limits** include:
 - Title or Author fields
 - Searching exact words or variants
 - Maximum number of results retrieved
 - Year of publication
 - Search by languages
 - o TOXLINE components

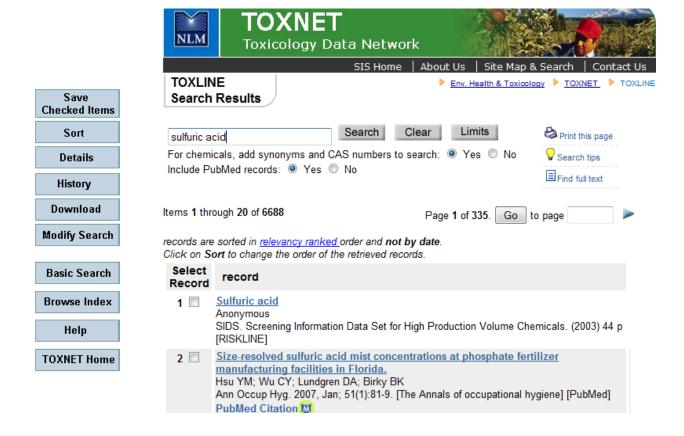


TOXLINE Results

 Citations that are also found in PubMed will be displayed with an icon that will link directly to PubMed



Each citation includes the database in brackets



Practice Exercise

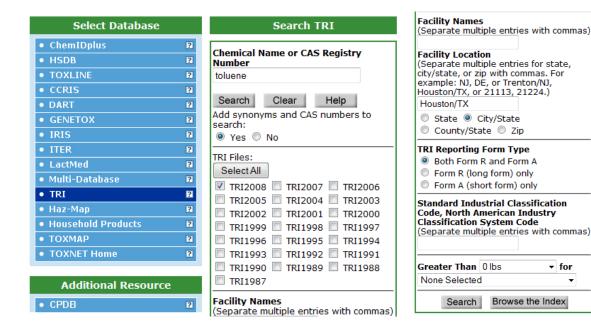
1.	Find citations to literature, journals or reports on environmental exposure
	to acetone in salons.

2. What are the effects of cocaine and alcohol usage on a fetus?

Toxic Releases Databases

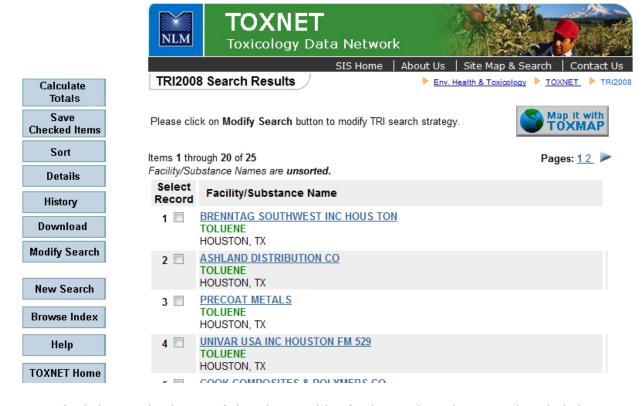
Toxics Release Inventory (TRI)

- Set of publicly available databases containing information on releases of specific toxic chemicals and their management as waste
- Based on data submitted to the EPA from industrial facilities in U.S.
- Describe the releases of toxic chemicals into the environment annually (1987 2008)
- Data includes names and addresses of facilities, the amounts of toxic chemicals released to the air, water, land, or transfer to waste sites
- Over 1.5 million records



- Search by chemical name or CAS number.
- Limit results to particular years, facilities, locations, Form type, SIC number and release amounts
- Browse the Index allows browsing by words, CAS numbers chemical names, facility names, or facility cities

- Results display in brief format with the facilities and chemical list
- The Map it with TOXMAP button displays the results in TOXMAP



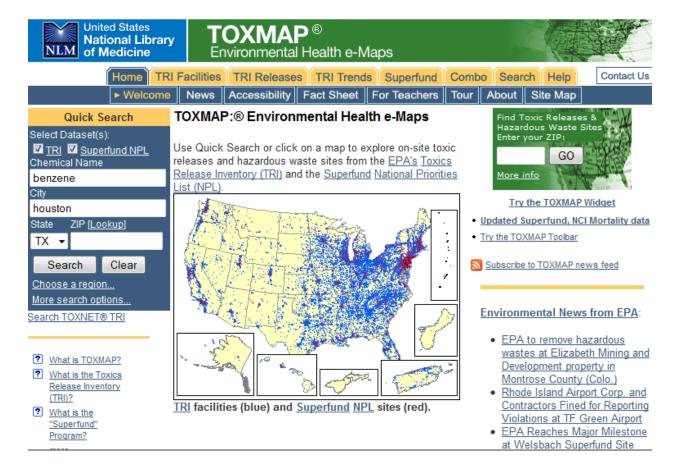
 To find the total release of the chemical by facility, select the record and click on Calculate Totals. Results summarize the total amount released

TRI Calculation Results



TOXMAP

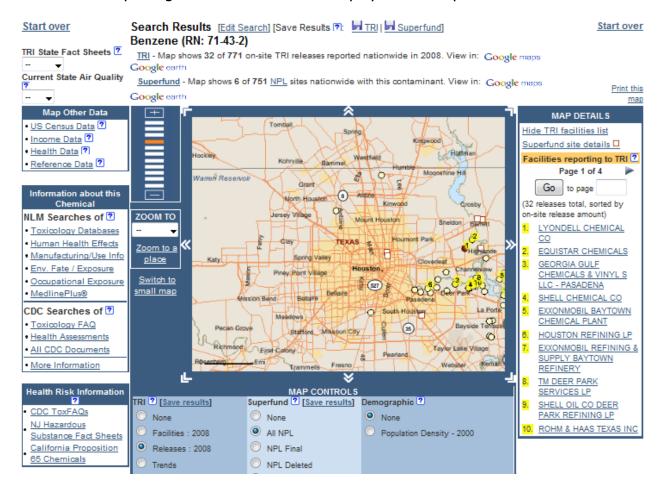
- From NLM
- Provides maps of the United States to help users visually explore data from the EPA's Toxic Releases Inventory (TRI) and the Superfund National Priorities List (NPL)
- Displays air, water, and land releases as reported by US industrial facilities
- Search by chemical name, facility name and/or location



- Trend a chemical released by facility or location
- Links to HSDB and ATSDR information as well as TOXLINE searches
- Can include census and reference data on map

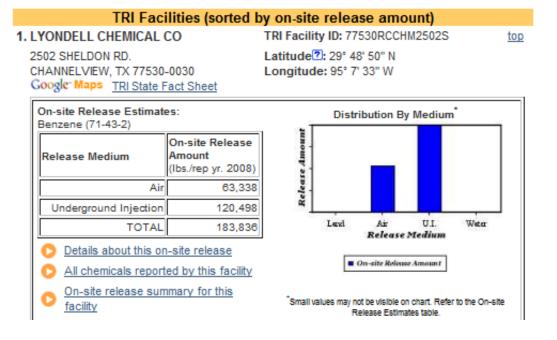
Searching TOXMAP

 To locate toxic releases in your area, type in your city and state into the quick search box and select the Go button Facilities reporting toxic releases will be displayed in a map



- **Map Other Data** adds more criteria to the results, such as US Census information, income data, health data and geography details
- Custom regional areas, such as several states can be created
- Information about this chemical links to other resources such as NLM and CDC databases are available
- Results may be viewed in Google Earth and Google Maps
- Map Controls and Legends are below the map
- To identify the specific facilities, click on the TRI on-site release details link under the Map Details section
- To access information on a particular facility, click on the facility's name

Details about other releases by this facility can be accessed



Other Databases

Haz-MAP

From NLM

High Risk Jobs

By Types of Jobs
 Alphabetically

- Occupational health database designed for health and safety professionals and for consumers seeking information about the health effects of exposure to chemicals and biological substances at work
- Search or browse by agents, diseases, jobs, and activities and processes, including non-occupational activities
- Contains over 5,500 chemicals and 225 occupational diseases



<u>Haz-Map:</u> Information on Hazardous Chemicals and Occupational Diseases by <u>Jay A. Brown, M.D., M.P.H.</u> Links to PubMed, TOXNET and other related resources

Haz Map Search Mo Browse Haz-Map	re Searches Y Haz Map Help Y Glossary Y References Search TOXNET		
Agent Name	Azure blue		
CAS Number	57455-37-5		
Formula	Unspecified		
Major Category	Dyes		
Synonyms	C. I. 77007; C.I. Pigment Blue 29; Pigment Blue 29; Ultramarine (pigment); Ultramarine Blue; Ultramarine blue pigment; [ChemIDplus]		
Category	Other Dyes		
Description	An inorganic, reddish-blue powder pigment and one of the three synthetic ultramarines; The structure is a "three-dimensional aluminosilicate lattice" containing ionic sulfur groups. Azure blue is "derived from china clay by calcination." [Ullmann]		
Sources/Uses	During the Middle Ages, ultramarine was used by artists as the "blue from over the sea." It was derived from the semiprecious stone, lapis lazuli, imported from Afghanistan. Since 1828 when it was first synthesized, the supply of the pigment has become abundant. Ultramarine pigments are used in plastics, paints, printing inks, paper, artist colors, laundry detergents (optical brightener), and toys. [Ullmann]		
Comments	"A nuisance dust." [Sax] Safe in manufacture and use with the only known hazard being the evolution of hydrogen sulfide after contact with acid; it is not irritating, sensitizing, or mutagenic; [Ullmann]		
	Links to Other NLM Databases		
Toxicity Information	Search TOXNET		
Chemical Information	Search ChemIDplus		
	Related Information in Haz-Map		
Processes	Industrial Processes with risk of exposure: • Painting (Pigments, Binders, and Biocides)		
Activities	Activities with risk of exposure: Painting		

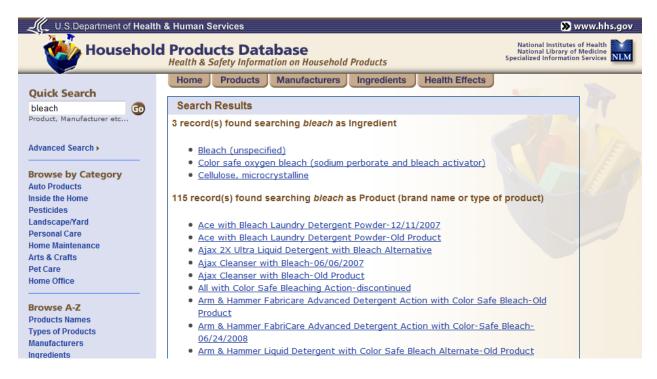
Household Products Database

- From NLM
- Information on potential health effects of chemicals or substances contained in more than 10,000 common household products
- Users can browse by a product category such as 'Pesticides' or by alphabetical listing of brand names
- Products can also be searched by type, manufacturer, product ingredient/chemical name and by health effects
- The complete Material Safety Data Sheets (MSDS) are available for products added since 2007
- Links to TOXNET, PubMed and other NLM databases



Searching Household Products Database

 To conduct a quick search, type in the name of the product, brand name or ingredient into the quick search box • Search results will include the search term as an ingredient and as a text word in the product name



- Select a record for more information about the product/item
- The detailed record includes information on the product, the manufacturer, health effects, handling/disposal, and ingredients
- Links within the record will access other NLM databases including PubMed and other TOXNET databases, and the MSDS (in some cases)



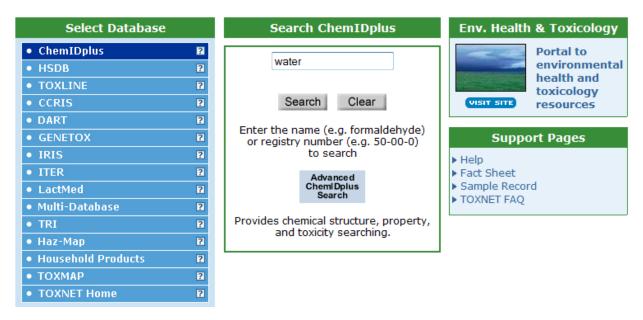
ChemIDplus

- Structure and name file used for the identification of chemical substances
- Contains over 378,000 chemical records, of which over 295,000 include chemical structures

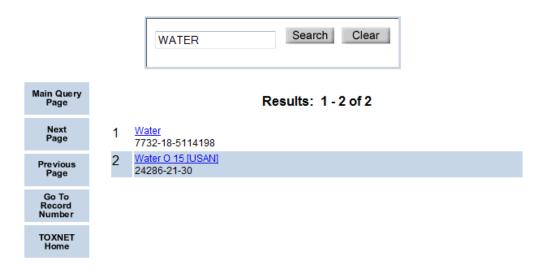
Basic Search

Search by substance name or CAS number

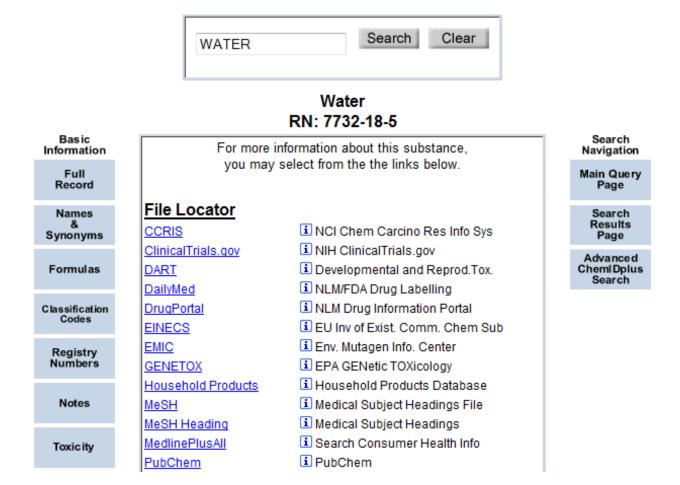
ChemIDplus - Dictionary of over 370,000 chemicals (names, synonyms, and structures). Includes links to NLM and other databases and resources.



- For most chemicals there is one record and the system automatically retrieves that record
- If multiple records are retrieved, a list of names will displayed



- The Basic Information buttons on the left of the results allow you to access the ChemIDplus Full Record, or a specific portion of the record, such as Names & Synonyms, Formulas, Classification Codes, Registry Numbers, Notes, Toxicity and Physical Properties
- The Search Navigation button on the right allows you to go back to a basic search (Main Query Page) or to the advanced search (Advanced ChemIDplus Search)



- The middle of the results page lists the **Locators** where further information on the chemical is found
- The **File Locators** point to NLM associated databases

Water RN: 7732-18-5

For more information about this substance. you may select from the the links below.

File Locator CCRIS i NCI Chem Carcino Res Info Sys i NIH ClinicalTrials.gov ClinicalTrials.gov DART i Developmental and Reprod. Tox. DailyMed NLM/FDA Drug Labelling DrugPortal i NLM Drug Information Portal i EU Inv of Exist. Comm. Chem Sub EINECS EMIC i Env. Mutagen Info. Center i EPA GENetic TOXicology GENETOX i Household Products Database Household Products MeSH i Medical Subject Headings File i Medical Subject Headings MeSH Heading MedlinePlusAll i Search Consumer Health Info PubChem i PubChem PubMed i Biomedical Citations From PubMed i AIDS Citations from PubMed PubMed AIDS i Cancer Citations from PubMed PubMed Cancer i Toxicology Citations From PubMed PubMed Toxicology RTECS i Reg. of Toxic Eff. of Chem. Sub. i NLM TOXLINE on TOXNET TOXLINE

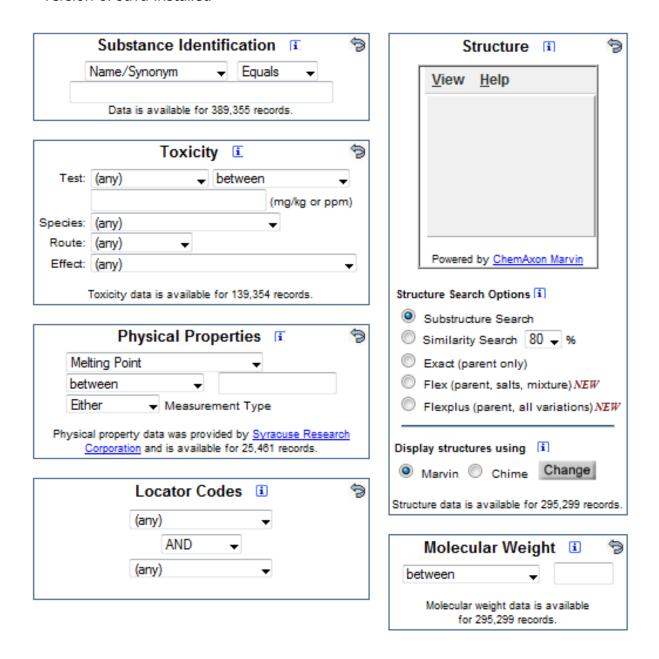
- Internet Locators link to web resources containing biomedical data
- Superlist Locators link to regulatory and scientific lists

Internet Locator	
CTD	i Comparative Toxicogenomics Database
ChEBI	i Chem Entities of Biological Interest
Drugs@FDA	i FDA Drug Database
EPA Envirofacts	i EPA Master Chemical Integrator
EPA HPVIS	i EPA High Prod Vol Info System
EPA SRS	i EPA Substance Registry System
IUCLID	i EU IUCLID Chemical Data Sheet
NIST WebBook	i NIST Chemistry WebBook
NTP DBS	i NTP Database Search
SRC CHEMFATE	i Syracuse Res. Corp. CHEMFATE
SRC DATALOG	i Syracuse Res. Corp. DATALOG
USA.gov	i USA.gov Search Engine
Superlist Locator	
CGB	i DOT Coast Guard Bulk Haz. Mat.
DSL	i Domestic Sub. List of Canada
INER	i EPA Pesticide Inert Ingredients
TSCAINV	i EPA Chem. Sub. Inventory

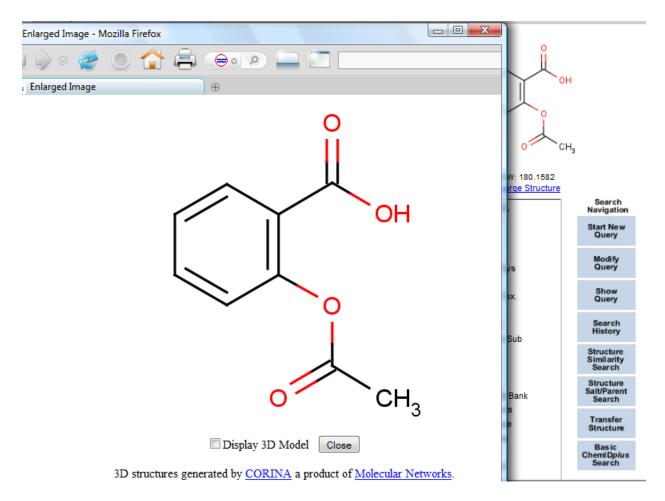
- Clicking on the Information icon information on the resource
- To view the results in any Locator, click on its name

Advanced Search (ChemIDplus Advanced)

- Search by chemical name, CAS number, molecular formula, classification code, locator code, structure or substructure, toxicity indicators, physical properties, and molecular weight
- Provides structural drawings that can be manipulated
- To use ChemIDplus Advanced, you will need a web browser that has a recent version of Java installed



 After clicking the Enlarge Structure link, you will be able to display a threedimensional model of the structure



 Structure Similarity, Structure Salt/Parent Search and Transfer Structure copies the structure into the Advanced Search and allows for structure searching

Practice Exercises

1.	Find the Mercury releases in Houston, Texas. Which facility has the highest amount of releases?
2.	What are the acute health effects associated with Victor Roach Killing Powder?
3.	Find the chemical structure for Furosemide